THE ASTROPHYSICAL JOURNAL, 270:L99–L100, 1983 July 15

LABORATORY MEASUREMENT OF THE $J = 2 \rightarrow 3$ ROTATIONAL TRANSITION FREQUENCY OF $HC^{17}O^+$

GRANT M. PLUMMER, ERIC HERBST, AND FRANK C. DE LUCIA
Department of Physics, Duke University
Received 1983 March 14; accepted 1983 March 29

ABSTRACT

The $J = 2 \rightarrow 3$ rotational transition frequency of $HC^{17}O^+$ has been measured to be 261,164.92(10) MHz by means of millimeter-wave spectroscopy. A combination of new and old data on the previously studied isotopes $HC^{16}O^+$ and $HC^{18}O^+$ has been used to redetermine the spectroscopic constants of $HC^{17}O^+$. Frequency predictions based on these newly determined $HC^{17}O^+$ constants are in excellent agreement with both our measurement and the probable measurement of the $J = 1 \rightarrow 0$ transition frequency in Sgr B2 (OH) by Guélin, Cernicharo, and Linke.

Subject headings: laboratory spectra — molecular processes

The laboratory study of the rotational transition frequencies of the formyl ion (HCO^+) and some of its isotopes has been undertaken by Woods and collaborators (Woods *et al.* 1975; Woods *et al.* 1981), Bogey, Demuynck, and Destombes (1982), and ourselves (Sastry, Herbst, and De Lucia 1981). In this *Letter*, we report the frequency of the $J = 2 \rightarrow 3$ transition of the ion $HC^{17}O^+$ which has not previously been detected in the laboratory. With our new magnetic field enhancement technique applied to an abnormal glow discharge (De Lucia *et al.* 1983), we have observed the $J = 2 \rightarrow 3$ transition using a gaseous mixture of H_2 and CO with *natural* isotopic abundance ratios.

Our measured $J = 2 \rightarrow 3$ $HC^{17}O^+$ transition frequency is 261,164.92(10) MHz. This value can be utilized to help confirm the recent attribution by Guélin, Cernicharo, and Linke (1982, hereafter GCL) of a line at 87,057.5 MHz in the Sgr B2 (OH) spectrum to the $J = 1 \rightarrow 0$ transition of $HC^{17}O^+$. GCL estimated the spectroscopic constants of $HC^{17}O^+$ from experimental data on $HC^{16}O^+$ and $HC^{18}O^+$. Use of their constants leads to a prediction of 261,165.5 MHz for the $J = 2 \rightarrow 3$ $HC^{17}O^+$ transition frequency and reproduces the frequency of the Sgr B2 line. There is some question, however, about the accuracy of the predicted $J = 2 \rightarrow 3$ frequency. According to the more conservative estimate of GCL, the accuracy should be ± 1.5 MHz. These authors found, however, that their method of estimating spectroscopic constants of ^{17}O-containing molecules by using ^{16}O and ^{18}O data is accurate to a few times 10^{-7} for well-studied molecules. By this criterion, the accuracy of the $J = 2 \rightarrow 3$ prediction should be $\sim \pm 0.1$ MHz, and the predicted and measured frequencies are in slight disagreement. This slight disagreement is removed when the $HC^{17}O^+$ spectroscopic constants used by GCL are refined based on a new $HC^{18}O^+$ measurement (see below).

An additional argument that the Sgr B2 species is the same as that measured in our laboratory stems from the size of the quadrupolar broadening of the spectra due to the quadrupole moment of the ^{17}O nucleus. Based on the quadrupole coupling constant eQq for $HC^{14}N$, GCL estimated eQq for $HC^{17}O^+$ to be 12 MHz, but they found little if any evidence of spectral broadening in the Sgr B2 spectral line and concluded that $eQq \leq 12$ MHz. We also find little if any evidence of broadening in the $J = 2 \rightarrow 3$ spectral line and infer a similar upper limit for eQq.

We have also observed in natural abundance the previously unmeasured $J = 2 \rightarrow 3$ transition frequency of $HC^{18}O^+$ and find it to be 255,479.389(20) MHz. With this frequency and previously measured laboratory values for the $J = 0 \rightarrow 1$ frequency (Woods *et al.* 1981) and $J = 1 \rightarrow 2$ frequency (Bogey, Demuynck, and Destombes 1982), we obtain the rotation (B_{000}) and centrifugal distortion (D_{000}) spectroscopic constants listed in Table 1. These constants, determined from a three-line spectrum, are expected to be more accurate than the earlier values of Bogey, Demuynck, and Destombes (1982) which were based on just two lines. Using our $HC^{18}O^+$ and $HC^{16}O^+$ (Sastry, Herbst, and De Lucia 1981) spectroscopic constants, we have utilized

TABLE 1

SPECTROSCOPIC CONSTANTS OF $HC^{18}O^+$ AND $HC^{17}O^+$

Constant	$HC^{18}O^+$ [a]	$HC^{17}O^+$ [b]
B_{000} (MHz)	42,581.281(46)	43,528.933
D_{000} (kHz)	76.6(3.1)	80

[a] Least squares fitted values.
[b] Determined via mass relations from $HC^{16}O^+$ and $HC^{18}O^+$ data.

the procedure outlined in GCL to obtain improved values of B_{000} and D_{000} for $HC^{17}O^+$. These values, listed in Table 1, lead to a $J = 1 \rightarrow 0$ transition frequency of 87,057.55 MHz and a $J = 2 \rightarrow 3$ transition frequency of 261,164.96 MHz, in excellent agreement with both astronomical and laboratory measurements. The evidence is therefore strong that the 87,057.5 MHz line observed by GCL in Sgr B2 (OH) has indeed been correctly attributed to the $J = 1 \rightarrow 0$ transition of $HC^{17}O^+$. Interstellar observation of the $J = 3 \rightarrow 2$ transition should serve to eliminate the possibility that the 87,057.5 MHz line can be attributed at least in part to a different species.

We wish to acknowledge the support of NASA via grant number NAGW-189. The aid of Dr. Paul Helminger and Mr. Geoffrey A. Blake in the measurement of the $HC^{18}O^+$ transition frequency is gratefully acknowledged.

REFERENCES

Bogey, J., Demuynck, C., and Destombes, J. L. 1982, *Molec. Phys.*, **43**, 1043.
De Lucia, F. C., Herbst, E., Plummer, G. M., and Blake, G. A. 1983, *J. Chem. Phys.*, **78**, 2312.
Guélin, M., Cernicharo, J., and Linke, R. A. 1982, *Ap. J. (Letters)*, **263**, L89 (GCL).
Sastry, K. V. L. N., Herbst, E., and De Lucia, F. C. 1981, *J. Chem. Phys.*, **75**, 4169.
Woods, R. C., Dixon, T. A., Saykally, R. J., and Szanto, P. G. 1975, *Phys. Rev. Letters*, **35**, 1269.
Woods, R. C., Saykally, R. J., Anderson, T. G., Dixon, T. A., and Szanto, P. G. 1981, *J. Chem. Phys.*, **75**, 4256.

FRANK C. DE LUCIA, ERIC HERBST, and GRANT M. PLUMMER: Department of Physics, Duke University, Durham, NC 27706